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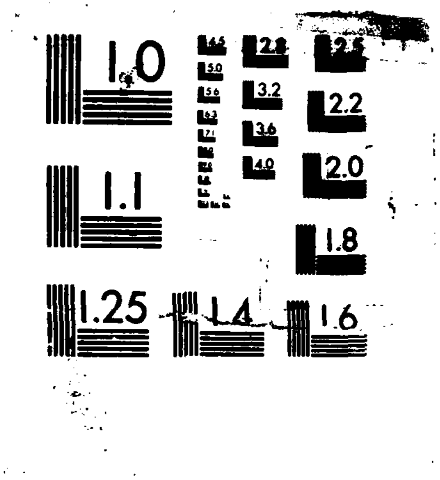

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This annual report summarizes Yale High Temperature Chemical Reaction Engrg. laboratory research methods/results (Grant AFOSR 84-0034) for the one-year period ending 11/30/85. Our techniques and results are outlined in the areas of (1) laser-based real-time optical techniques for measuring vapor and/or particle-deposition rates onto cooled surfaces in combustion gases, (2) role or thermophoresis in the capture of soot particles andthe useof this phenomenon to infer both local soot volume fractions and local gas temperatures, (3) boundary layer computational methods and correlation for thermophoretically-modified small particle transport, including high mass-loading effects, and (4) use of a micro-wave-induced plasma emissiom emission spectroscopic (MIPES) method to follow boron surface sublimation and gasification kinetics in stream containing $O_2(g)$ or $CO_2(g)$. Presentations and publications describing these techniques/findings are documented. Keywords;

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1. INTRODUCTION

The performance of ramjets burning slurry fuels (leading to condensed oxide aerosols and liquid film deposits), gas turbine (GT) engines in dusty atmospheres, or when using fuels from non-traditional sources (e.g., shale-, or coal-derived), depends upon the formation and transport of small particles across non-isothermal combustion gas boundary layers (BLs). Moreover, even airbreathing engines burning "clean" hydrocarbon fuels can experience soot formation/deposition problems (e.g., combustor liner burnout, accelerated turbine blade erosion and "hot" corrosion). Accordingly, our research is directed toward providing chemical propulsion systems R & D engineers with new techniques and quantitative information on important particle and vapor mass transport mechanisms and rates.

The purpose of this report is to briefly summarize our research methods and accomplishments under AFOSR Grant 84-0034 (Technical Monitor: J.M. Tishkoff) during the one-year period: 12/1/84 - 11/30/85. Readers interested in greater detail than contained in Section 2 are advised to consult the published papers cited in Sections 2, 5. Copies of any of these published papers or preprints can be obtained by writing the PI: Prof. Daniel E. Rosner at the Department of Chemical Engineering, Yale University, Box 2159 Yale Station, New Haven, CT 06520, U.S.A. Comments on, or examples of, the applicability of our research results will be especially welcome.

An interactive experimental/theoretical approach is being used to gain an understanding of performance-limiting chemical-, and mass/energy transfer-phenomena at or near interfaces. This includes the development and exploitation of seeded laboratory flat flame burners and cooled deposition targets (see, e.g., Fig. 1), flow-reactors (Fig. 8), and new optical diagnostic/ spectroscopic techniques. Resulting experimental rate data, together with the predictions of comprehensive asymptotic theories, are then used as the basis for proposing and verifying simple viewpoints and effective engineering correlations for future design/optimization studies.

2. RESEARCH ACCOMPLISHMENTS AND PUBLICATIONS

Most of the results we have obtained under Grant AFOSR 84-0034 can be subdivided into the 3 sub sections below:

2.1 Seeded Flame Experiments on Vapor and Submicron Particulate Transport Rates

Using seeded, atmospheric pressure flat flame burner techniques (1,10,14) combined with the laser optical probing of chemically inert, reflective targets (e.g., Pt ribbons; see Fig. 1) we have studied the rates of chemical vapor deposition (14), submicron particle deposition (1) and the rates of condensate evaporation (e.g., $B_2O_3(\ell)$; see Fig. 2 and Section 3). In unseeded but fuel-rich hydrocarbon/oxygen flames we have demonstrated that carbonaceous soot particle transport to immersed thermocouple probes occurs according to the laws of thermophoresis (4,5). Thus, straight-line re-plots of thermocouple diameter vs. time data are possible (Fig. 3) and the slopes (m) of these particular plots, presumably proportional to the local soot volume fraction $f_{v,e}$, are indeed consistent with laser light extinction measurements across these same flames (Fig. 4). According to the same theory, it should also be possible to simultaneously determine local gas temperatures — a scheme which we call "thermophoretic thermometry". One variant, currently under investigation, is sketched in Fig. 5, where the notation is that of Ref. 4 and $\mathscr{K}$ is $d \ln k_g / d \ln T$, where k_g is the combustion gas thermal conductivity. Ironically, in this scheme the presence of soot is exploited to determine T_g, and is not the obstacle which greatly complicates its accurate inference (4)!

2.2. Transport Theory: Thermophoretically Modified Boundary Layer Convective Mass Transport

We are extending our previous solutions and correlations of thermophoretically modified submicron particle mass transport across laminar (3,7,8) and turbulent BLs (6,8) into the domain of high particle mass loading (16), a situation encountered in numerous materials processing applications, and, locally, in two-phase (e.g., droplet/gas) flows of chemical propulsion interest. Also, because of increasing interest in the Soret diffusion of large, highly nonspherical molecules and the thermophoretic transport of nonspherical particles (e.g., long soot aggregates) we have recently predicted their thermal diffusion factors, α_T, (Fig. 6, Ref. 15) and hope to experimentally test some of these predictions and their BL-consequences in the future. We have also begun exploring the scavenging effects of submicron particulate matter (e.g., an inorganic mist or fume) on vapor diffusion across BLs (12), using a mathematical model in which the departure from local vapor/liquid equilibrium is dictated primarily by the product of a Damköhler number (C) and particle loading parameter (L) (see Fig. 7). These methods/results, along with our previous analysis of shear-driven viscous deposits (17), could be used to predict the behavior of reaction product "glass" layers on turbine blades and/or exhaust nozzles, as well as the behavior of glass-forming refractory solids in high-shear corrosive multiphase environments.

2.3. Heterogeneous Kinetics

To make (i) rapid-response gas/solid reaction rate measurements over a large temperature range, and (ii) surface mass balances necessary for mechanistic understanding of high temperature gas/solid reactions, we have recently been exploiting an emission spectroscopic technique. In this technique, a low pressure microwave-induced plasma (MIP) excites characteristic emission from the atoms in the gaseous product species of a gas/solid reaction in a low pressure flow reactor.

We employ a modified version of our transonic, vacuum flow reactors (Fig. 8) developed earlier under AFOSR-support for the study of gas reactions with silicon- and boron-containing refractory solid compounds (18). However, now the reaction product vapor species are dissociated and electronic emission from the resulting atoms is produced in a microwave discharge plasma (G) before leaving the reactor. Evaporation and gasification reactions are studied by measuring emission intensity, I, from this discharge, via a 0.5m Jarrell-Ash monochromator.

Aside from steady-state reaction rate measurements, flash evolution experiments can be carried out to measure the amount of condensed product material formed on a surface during reaction, provided, of course, that the reaction product (e.g., B_2O_3) has a higher volatility than that of the substrate, e.g., B(s). In such experiments the filament is exposed to the gaseous reagent for some reaction time (normally only a few minutes). Then, the gaseous reagent flow into the reactor is stopped and the filament cooled. Finally, the I(t) is determined when the filament is heated rapidly. The skimmer and the inner co-axial tube shown in Fig. 8 were installed so that the system detects only products from the central, uniform-temperature region of the filament.

We are now performing preliminary experiments on the application of this microwave-induced plasma emission spectroscopy (MIPES) technique to the oxidation of boron, a system of considerable interest to the propulsion community, but one whose poorly understood kinetics are apparently influenced by the condensibility of the reaction product B_2O_3. Preliminary results have been obtained for the high temperature gasification kinetics of boron by $O_2(g)$, and $CO_2(g)$, and will be reported at the next Eastern States Combustion Institute Conference. In the future we will initiate measurements of the oxidation kinetics of boron by $B_2O_3(g)$ (i.e., OBOBO(g)) and exploit the rapid-response characteristics of our MIPES technique to measure the behavior of such surfaces in modulated reactant streams. Among other things, such studies could shed valuable light on the response of solid fuel surfaces in a turbulent environment.

3. ADMINISTRATIVE INFORMATION ; PERSONNEL AND PRESENTATIONS

Table 3.1 summarizes the personnel who have contributed to this research program during the period: 12/1/84 - 11/30/85, along with the subject matter of each investigator's research contribution.

Table 3.1

SUMMARY OF PERSONNEL AND THEIR CONTRIBUTIONS

Name	Status @ Yale	Primary Contribution
Rosner, D.E.	PI[a], ChE	Overall Program Direction[19]
Eisner, A.D.	PDRA (thru 6/7/85)	Soot deposition from flames[4,5]
Gomez, A.	PDRA[c] (starting 9/85)	Experimental determination of $\alpha_T D_p$
Garcia-Ybarra, P.	PDRA	Thermophoretical properties of nonspherical particles[15]
Liang, B.	GRA[b] (87)	Vapor and/or particle deposition interaction[10]
Naragajan, R.	GRA (86)	Dynamics of C.V.D. condensate layers[17]
Park, H.M.	GRA (87)	Theory of high-mass-loaded aerosol transport[16]
Roy, R.	GRA (MA)	Thermodynamics of nonideal condensate mixtures
Tanoff, M.	GRA	Experimental determination of $\alpha_T D_p$

[a] Principal Investigator
[b] Graduate Research Assistant (Anticipated Year of PhD Degree)
[c] Postdoctoral Research Assistant

Table 3.2.

SUMMARY OF TALKS[a] BASED IN PART ON OSR-GRANT

Date	Host Organization	Location	Topic(s)
12/16-21/84	Phys. Chem. Hydrodyn. No5[b] (Levich)[9]	Tel Aviv, Israel	2.2
2/18/85	Univ. Pennsylvania, ChE Dept.	Philadelphia, PA	2.1, 2.2
8/5/85	ASME/AIChE Heat Transfer Conference[19]	Denver, Colorado	2.2
9/18/85	Cambridge Univ., ChE Dept.	Cambridge, U.K.	2.1, 2.2
9/27/85	Sheffield Univ., ChE Dept.	Sheffield, U.K.	2.1, 2.2
10/2/85	CEGB-Marchwood Lab.	Southampton, U.K.	2.1, 2.2
10/16/85	Technion-Israel Inst. Techn., Dept. Aero. Engrg.	Haifa, Israel	2.2
10/23/85	Technion IIT, Dept. ChE	Haifa, Israel	2.1
11/12/85	ENSIC-CNRS	Nancy, France	2.3
11/18/85	Combustion/High Temp. Res. Ctr. CNRS	Orleans, France	2.1, 2.2
11/19-22/85	American Assoc. Aerosol Research[b]	Albuquerque, NM	2.2
11/23/85	City Univ., Dept. Aero. Engrg.	Madrid, Spain	2.1, 2.2
11/26/85	Polytechnic Univ. Seville	Seville, Spain	2.1, 2.2
11/28/85	U.N.E.D., Dept. Fund. Phys.	Madrid, Spain	2.1, 2.2

[a] Presented by D.E. Rosner (unless otherwise specified)
[b] Presented by Dr. A. Eisner

4. CONCLUSIONS, FUTURE RESEARCH

In the OSR-sponsored work briefly described here we have shown that new laser-based experimental techniques for rapidly measuring vapor- and particle-mass transfer rates (1,5,14), combined with recent advances in what might be called "thermophoretic boundary layer theories" (2,3,6-9,19), are providing useful means to incorporate these phenomena in many propulsion engineering design/optimization calculations. In the future we hope to extend this work to include, among other things, the potentially important effects of high local particle mass loading (16), non-negligible particle <u>inertia</u>, and highly nonspherical particles (or molecules) (15). To shed light on particle ignition, "steady" combustion and extinction, our current research on the kinetics of boron gasification using MIPES will be extended to examine the $B_2O_3(g)/B(s)$ reaction and the response of such surfaces to sudden changes in temperature and reactant partial pressures.

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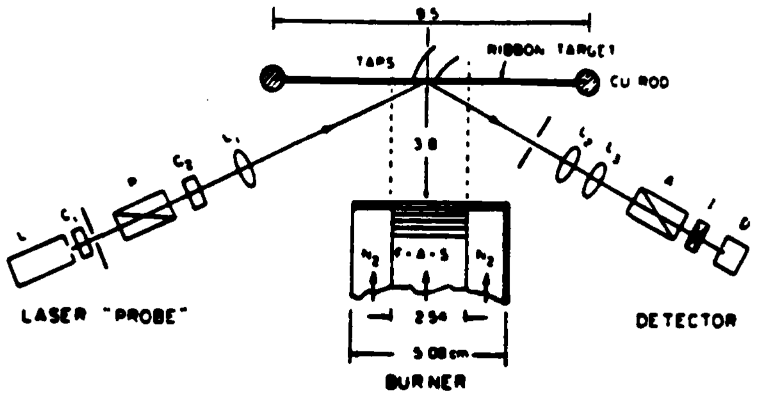

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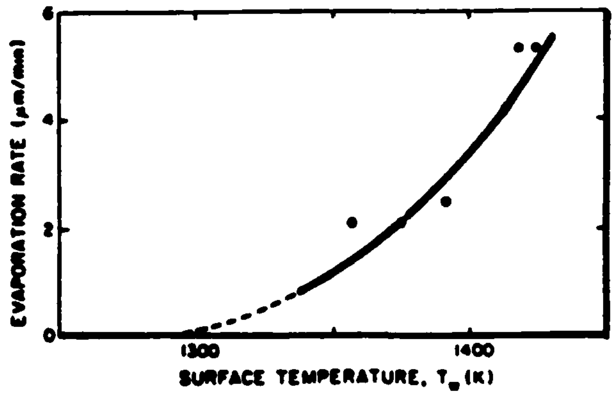

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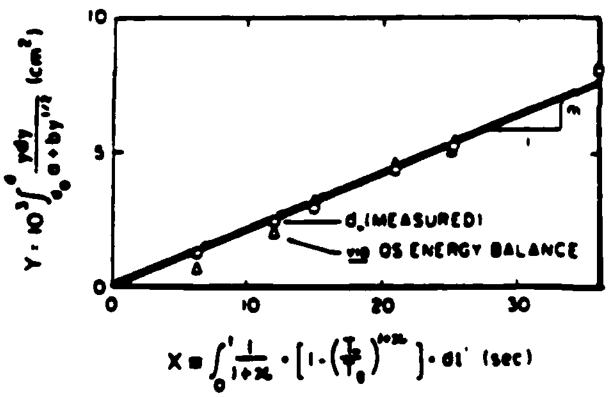

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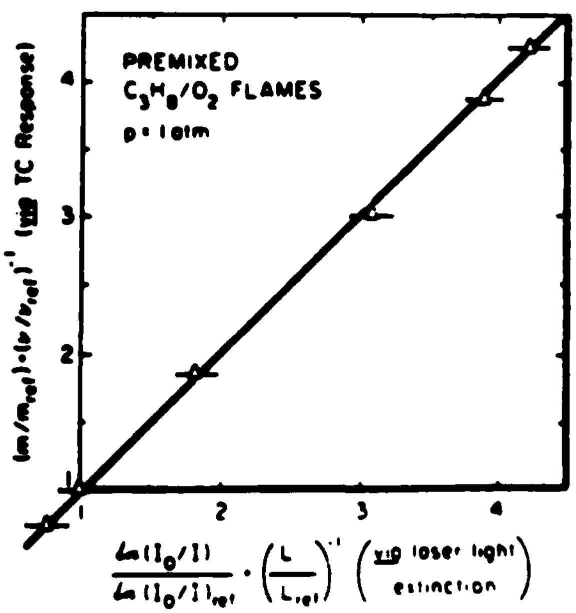

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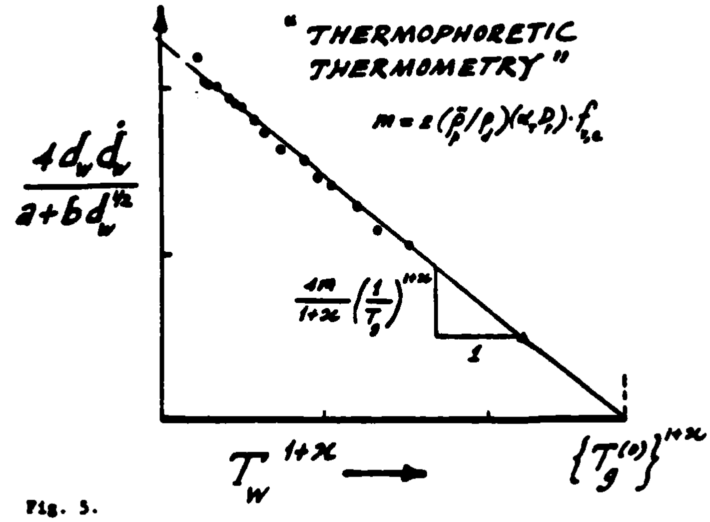

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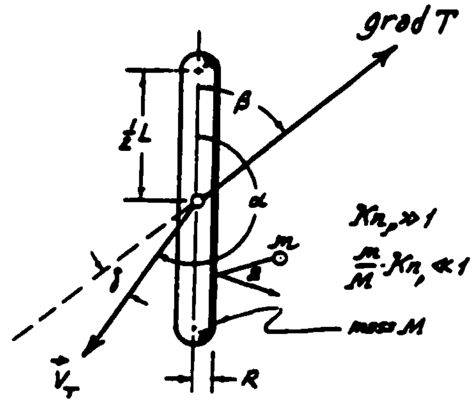

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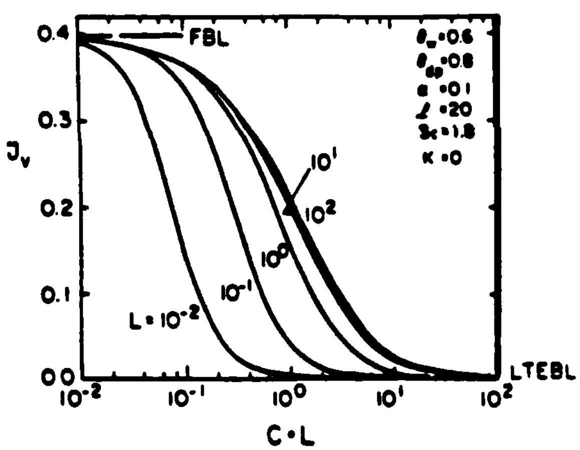

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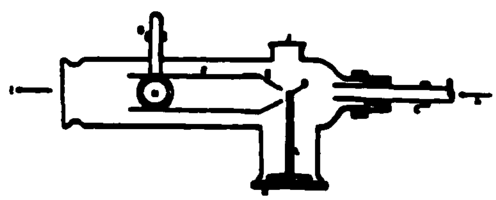

A, reactant and inert gas mixture. B, alumina tube. C, microwave cavity. D, electrically heated specimen filament. E, aluminum skimmer. F, pyrex annular tube. G, microwave cavity. H, quartz observation window. I, to pump, manometer, and throttle valve. J, pyrometer sight tube. K, specimen probe. L, electrical leads and voltage taps to measure specimen resistance

Fig. 8.

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